

Chapter 2

ATOMIC STRUCTURE AND INTERATOMIC BONDING

Chapter 2: Main Concepts

1. History of atomic models: from ancient Greece to [Quantum mechanics](#)
2. Quantum numbers
3. **Electron configurations** of elements
4. **The Periodic Table**
5. *Bonding Force and Energies*
6. **Electron structure and types of atomic bonds**
7. Additional: How to see atoms: [Transmission Electron Microscopy](#)

Topics 1, 2 and partially 3: Lecture 3

Topic 5: Lecture 4

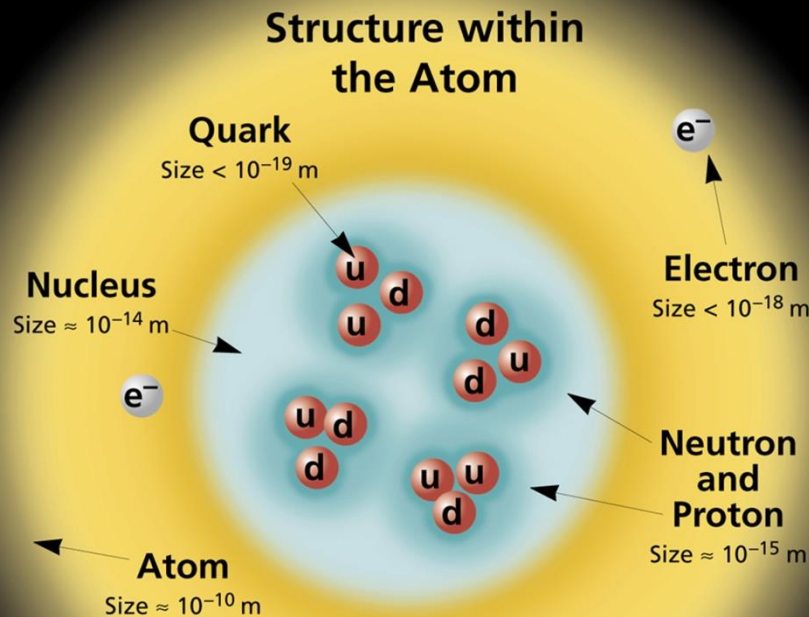
Topic 7: Lecture 5

Topics 4&6: self-education (book and/or WileyPlus)

Question 1: What are the different levels of Material Structure?

- *Atomic structure* ($\sim 1 \text{ Angstrom} = 10^{-10} \text{ m}$)
- *Crystalline structure* (short and long-range atomic arrangements; 1-10 Angstroms)
- *Nanostructure* (1-100nm)
- *Microstructure* (0.1 -1000 μm)
- *Macrostructure* ($>1000 \mu\text{m}$)

Q2: How does atomic structure influence the Materials Properties?



If the protons and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 mm in size and the entire atom would be about 10 km across.

- In general atomic structure defines the ***type of bonding*** between elements
- In turn the bonding type (ionic, metallic, covalent, van der Waals) ***influences the variety of materials properties*** (module of elasticity, electro and thermal conductivity and etc.).

MATERIALS CLASSIFICATION

Representative examples, applications, and properties for each category of materials

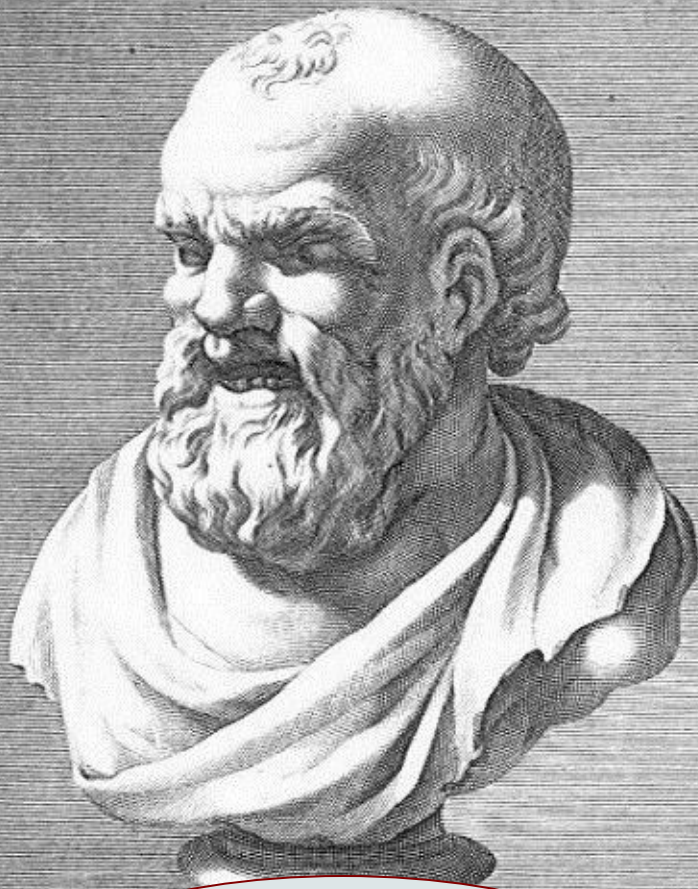
	Examples of Applications	Properties
Metals and Alloys		
Copper	Electrical conductor wire	High electrical conductivity, good formability
Gray cast iron	Automobile engine blocks	Castable, machinable, vibration-damping
Alloy steels	Wrenches, automobile chassis	Significantly strengthened by heat treatment
Ceramics and Glasses		
SiO ₂ -Na ₂ O-CaO	Window glass	Optically transparent, thermally insulating
Al ₂ O ₃ , MgO, SiO ₂	Refractories (i.e., heat-resistant lining of furnaces) for containing molten metal	Thermally insulating, withstand high temperatures, relatively inert to molten metal
Barium titanate	Capacitors for microelectronics	High ability to store charge
Silica	Optical fibers for information technology	Refractive index, low optical losses
Polymers		
Polyethylene	Food packaging	Easily formed into thin, flexible, airtight film
Epoxy	Encapsulation of integrated circuits	Electrically insulating and moisture-resistant
Phenolics	Adhesives for joining plies in plywood	Strong, moisture resistant
Semiconductors		
Silicon	Transistors and integrated circuits	Unique electrical behavior
GaAs	Optoelectronic systems	Converts electrical signals to light, lasers, laser diodes, etc.
Composites		
Graphite-epoxy	Aircraft components	High strength-to-weight ratio
Tungsten carbide-cobalt (WC-Co)	Carbide cutting tools for machining	High hardness, yet good shock resistance
Titanium-clad steel	Reactor vessels	Low cost and high strength of steel, with the corrosion resistance of titanium

- For example, five groups of materials can be outlined based on **structures and properties**:
 - metals and alloys
 - ceramics and glasses
 - polymers (plastics)
 - semiconductors
 - composites



Historical Overview

A-tomos



Democritus
460--~370 BC

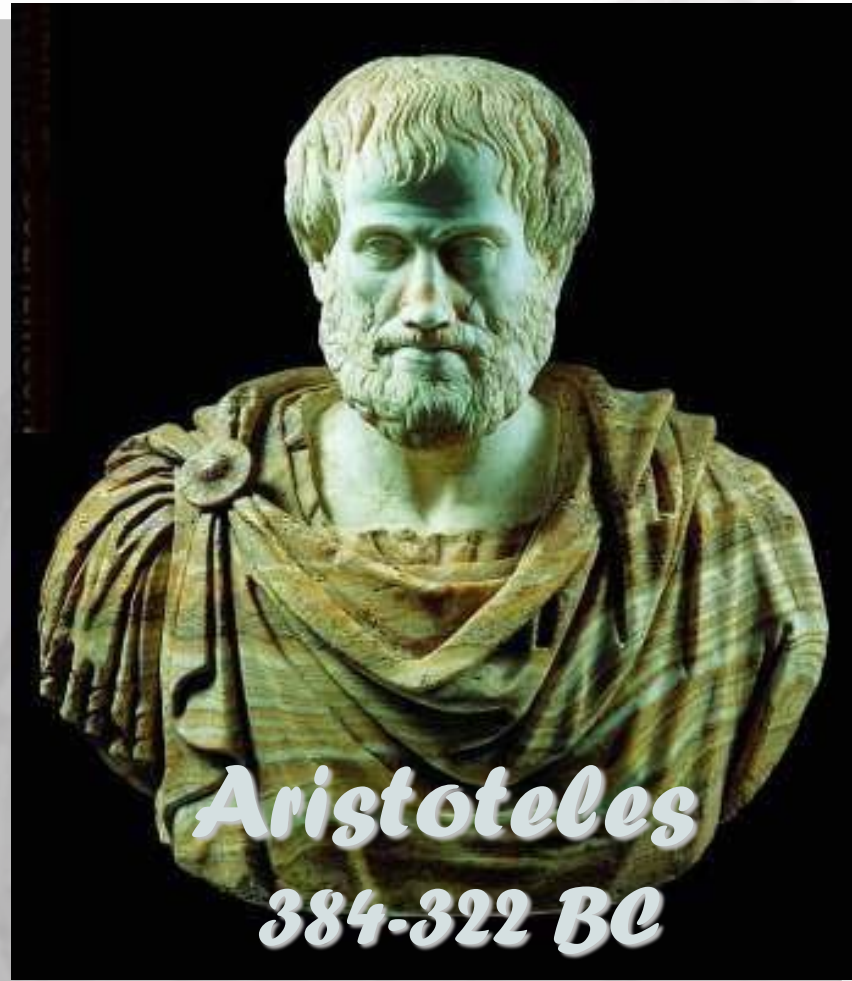
Ex marmore antiquo apud J. E.



On philosophical grounds:

There must be a smallest indivisible particle.

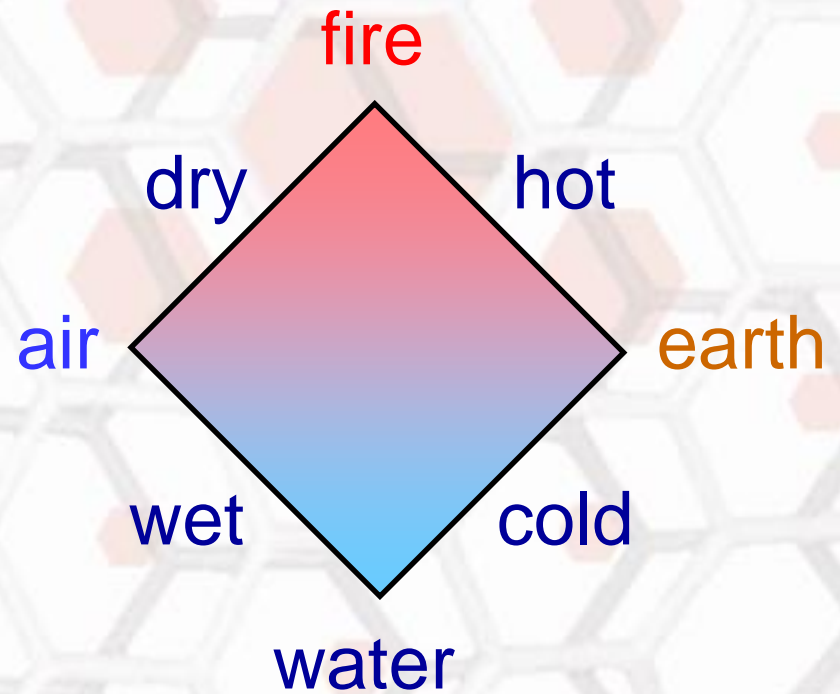
Arrangement of different particles at micro-scale determine properties at macro-scale.



Aristoteles
384-322 BC

Founder of **Logic** and
Methodology as tools for
Science and **Philosophy**

*It started
with ...*



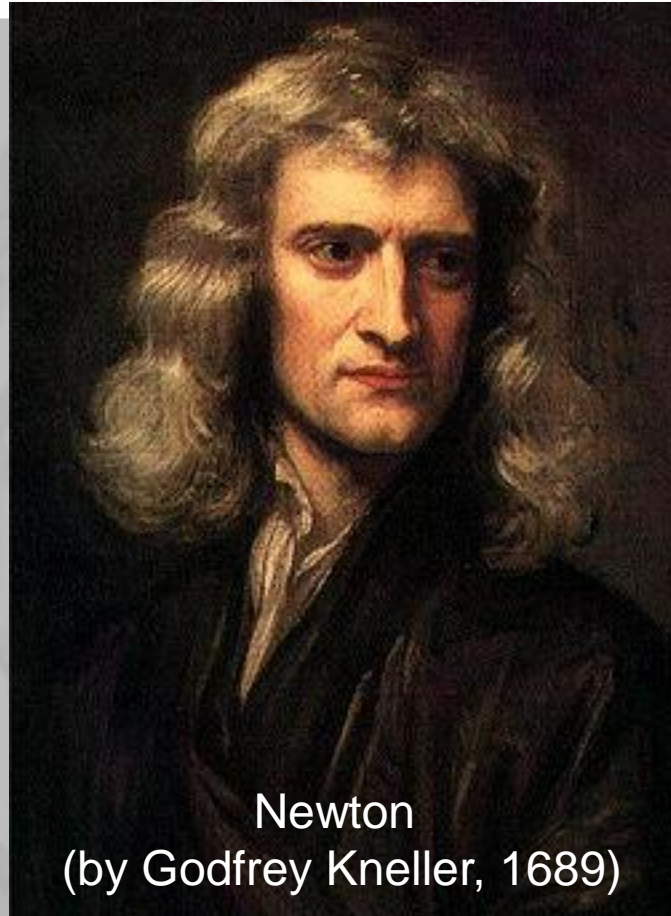
**The four elements
from ancient times**

Science?

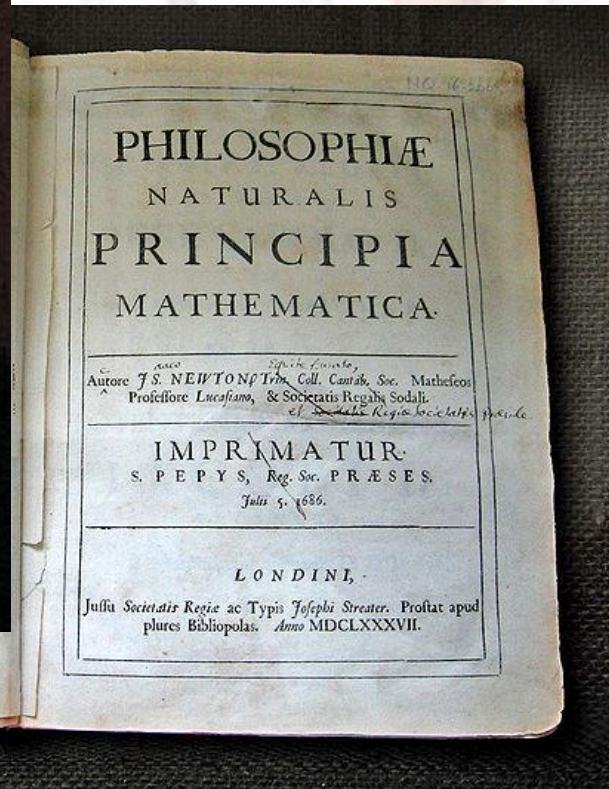
Newton published in 1687:
**'Philosophiæ Naturalis
Principia Mathematica'**,

**Newton !
(1643-1727)**

**... while the alchemists were
still in the 'dark ages'.**



**Newton
(by Godfrey Kneller, 1689)**



**Origin of classical
mechanics**

Gravitational force

**Movement of the
planets**

Atomic weights:
more clarity with the
help of physics.

Berzelius!

	1814	1818	1826	Modern
O	16	16	16	16
S	32.16	32.19	32.19	32.07
P	26.80	31.88x2	31.38x2	30.98
*M	22.33	22.82	--	--
Cl	--	--	35.41	35.46
C	11.99	12.05	12.23	12.01
H	1.062	0.995	0.998	1.008



*M = 'Murium', an unknown element that, together with oxygen, forms 'HCl' (muriatic acid, 'HMO').

Regularities in atomic weights

Triades !!!

1817: **Johann Dobereiner**
(and others) noticed
relations between atomic
weights of similar elements:

$$\text{Li} = 7$$

$$\text{Na} = 7 + 16 = 23$$

$$\text{K} = 23 + 16 = 39$$

$$\text{Mg} = 12$$

$$\text{Ca} = 12 + 8 = 20$$

$$\text{Sr} = 20 + 24 = 44$$

$$\text{Ba} = 44 + 24 = 68$$

Dumas (1851):

$$\text{N} = 14$$

$$\text{P} = 14 + 17 = 31$$

$$\text{As} = 14 + 17 + 44 = 75$$

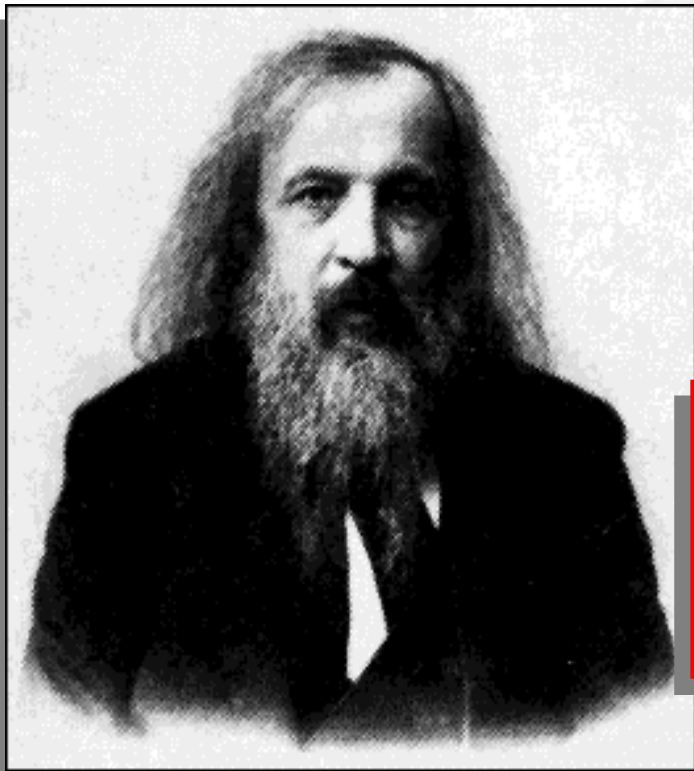
$$\text{Sb} = 14 + 17 + 88 = 119$$

$$\text{Bi} = 14 + 17 + 176 = 207$$

Also 'lateral relations' were
observed:

$$\text{Cl} - \text{P} = \text{Br} - \text{As} = \text{I} - \text{Sb} = 5$$

This led eventually to ...

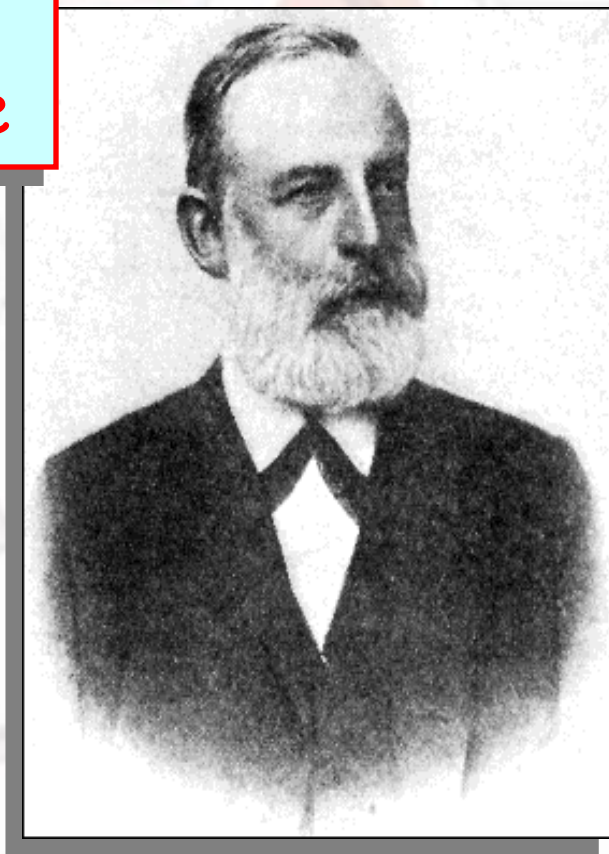


Mendeleëff

Start of the
modern
Periodic Table

Mendeleev and simultaneously
Meyers: ordering according to atomic
weights and similar properties.

Based on his system Mendeleev
did correct predictions of still
unknown, missing elements.

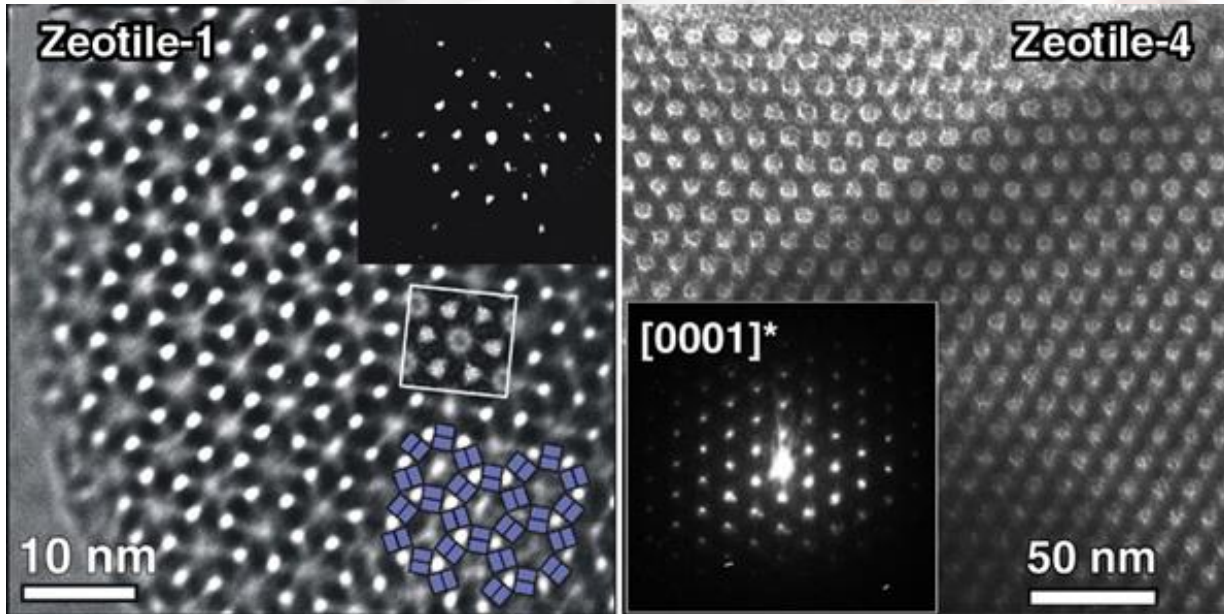


Atomic weights, not atomic numbers!

The original

Reihen	Gruppe I. - R ² O	Gruppe II. - RO	Gruppe III. - R ² O ³	Gruppe IV. RH ⁴ RO ²	Gruppe V. RH ³ R ² O ⁵	Gruppe VI. RH ² RO ³	Gruppe VII. RH R ² O ⁷	Gruppe VIII. - RO ⁴
1	<u>H</u> = 1							
2	<u>Li</u> = 7	<u>Be</u> = 9,4	<u>B</u> = 11	<u>C</u> = 12	<u>N</u> = 14	<u>O</u> = 16	<u>F</u> = 19	
3	<u>Na</u> = 23	<u>Mg</u> = 24	<u>Al</u> = 27,3	<u>Si</u> = 28	<u>P</u> = 31	<u>S</u> = 32	<u>Cl</u> = 35,5	
4	<u>K</u> = 39	<u>Ca</u> = 40	<u>-</u> = 44	<u>Ti</u> = 48	<u>V</u> = 51	<u>Cr</u> = 52	<u>Mn</u> = 55	<u>Fe</u> = 56, <u>Co</u> = 59 <u>Ni</u> = 59, <u>Cu</u> = 63
5	(<u>Cu</u> = 63)	<u>Zn</u> = 65	<u>-</u> = 68	<u>-</u> = 72	<u>As</u> = 75	<u>Se</u> = 78	<u>Br</u> = 80	
6	<u>Rb</u> = 85	<u>Sr</u> = 87	? <u>Yt</u> = 88	<u>Zr</u> = 90	<u>Nb</u> = 94	<u>Mo</u> = 96	<u>-</u> = 100	<u>Ru</u> = 104, <u>Rh</u> = 104 <u>Pd</u> = 106, <u>Ag</u> = 108
7	<u>Ag</u> = 108	<u>Cd</u> = 112	<u>In</u> = 113	<u>Sn</u> = 118	<u>Sb</u> = 122	<u>Te</u> = 125	<u>I</u> = 127	
8	<u>Cs</u> = 133	<u>Ba</u> = 137	? <u>Di</u> = 138	? <u>Ce</u> = 140	-	-	-	- - - -
9	(-)	-	-	-	-	-	-	
10	-	-	? <u>Er</u> = 178	? <u>La</u> = 180	<u>Ta</u> = 182	<u>W</u> = 184	-	<u>Os</u> = 195, <u>Ir</u> = 197, <u>Pt</u> = 198, <u>Au</u> = 199
11	(<u>Au</u> = 199)	<u>Hg</u> = 200	<u>Tl</u> = 204	<u>Pb</u> = 207	<u>Bi</u> = 208	-	-	
12	-	-	-	<u>Th</u> = 231	-	<u>U</u> = 240	-	- - - -

“Modern History“



- (1) The grain-like “indivisible” **spices** of Greek philosopher Democritus
- (2) *The **Rutherford-Chadwick** Model of the Atom*
- (3) **Bohr's model** of electron orbiting the nucleus
- (4) **Schrödinger's quantum** mechanical model of atom



Ernest Rutherford
1871-1937



Sir James Chadwick
1891-1974



Niles Bohr
1885-1962



Erwin Schrödinger
1887-1961

The Rutherford-Chadwick Planetary Model of the Atom



**Orbiting
electrons**

**The nucleus:
positively charged protons
and neutral particles-neutrons**

- Atoms = nucleus (***protons*** and ***neutrons***) + ***electrons***
- Protons and neutrons have almost the same mass, **$1.67 \times 10^{-27} \text{ kg}$** .
- Mass of an electron is much smaller, **$9.11 \times 10^{-31} \text{ kg}$**
- Protons and electrons positive and negative charges of the same magnitude, **$1.6 \times 10^{-19} \text{ Coulombs}$** , while neutrons are electrically neutral.

Model Summary

- **Atom**, which means “indivisible” in Greek, has an internal structure !!

Atom=nucleus [**protons** (p) and **neutrons** (n)] + **electrons** (e)

- $m_e = (9.109965 \pm 0.000014) \times 10^{-31}$ kg
- $m_p = (1.67482 \pm 0.00008) \times 10^{-27}$ kg
- $m_n = (1.67252 \pm 0.00008) \times 10^{-27}$ kg

$$m_p \approx m_n \gg m_e$$

The atomic mass (A) $\approx m_p + m_n$

- $Z_e = Z_p = (1.60210 \pm 0.000013) \times 10^{-19}$ Coulombs
- $Z_n = 0$

Atom is neutral

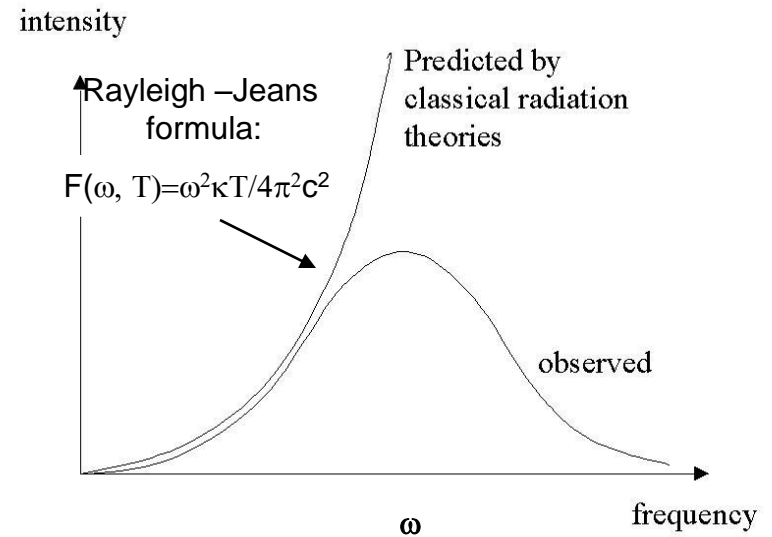
The atomic number (Z) = Number of protons (or electrons) in the atom

The atom **isotope number** is defined by Number of neutrons

Obstacle #1

The thermal motion of electrons and the thermal motion of ions relative to each other lead (due to Maxwell equations), to electromagnetic radiation as mentioned above. This is called **thermal radiation**.

Physicist tried to understand how the intensity of thermal radiation depends on frequency. Experimentally obtained results seemed to refuse to fit the calculations. The theory predicted higher contribution from higher frequencies but the reality was that the intensity dropped drastically at higher frequencies.



$$U(T) = \int \omega^2 \kappa T / 4\pi^2 c^2 = \infty$$

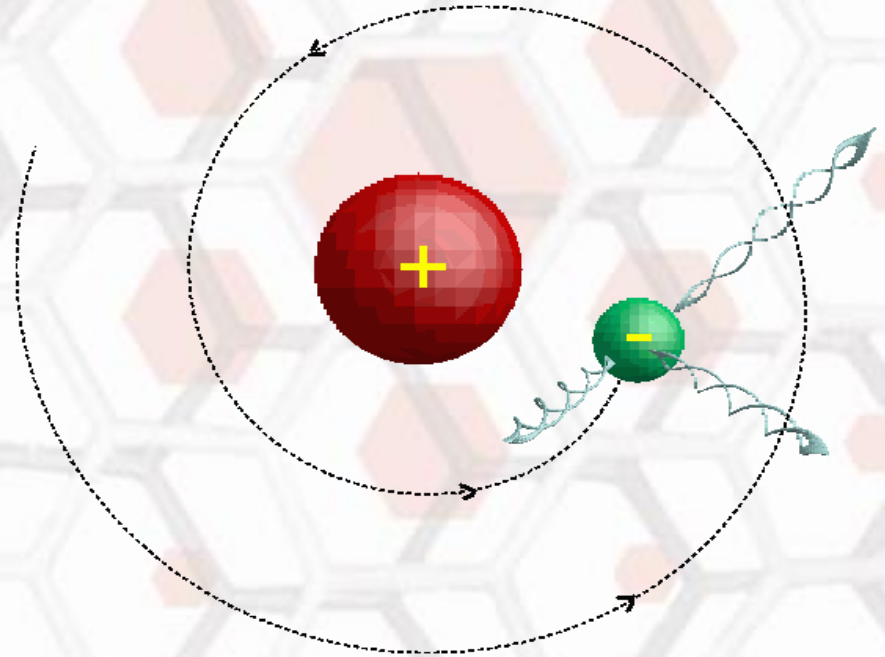
ultra-violet catastrophe !!

Obstacle #2

The most serious obstacles with the planetary model is that an orbiting electron has a centripetal **acceleration** and, according to *Maxwell's theory* of electromagnetism, ought to **lose energy** by emitting electromagnetic radiation at a frequency equal to that of the orbital motion.

The radiated energy would be at the expense of the electrostatic *potential* energy of the electron, thus the electron approaches closer to the nucleus and experiences an increased electrostatic force.

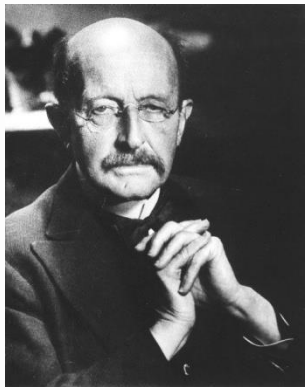
It leads to increase of angular velocity of the orbiting electron; the frequency of the emitted radiation would also increase and the electron would **spiral into the nucleus**.



Calculations showed that collision between electron and nucleus should happen in a **small fraction of a second**, thus atom should **not be stable !!**

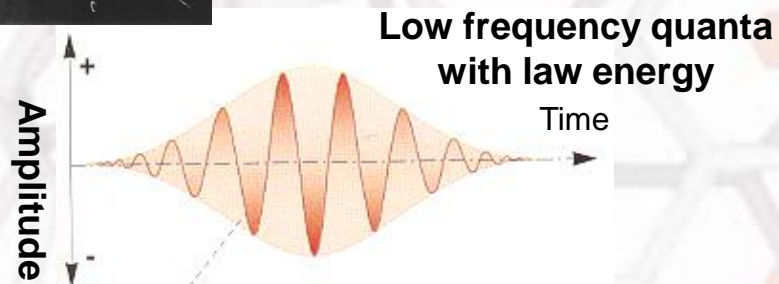


Quantum Mechanical Model

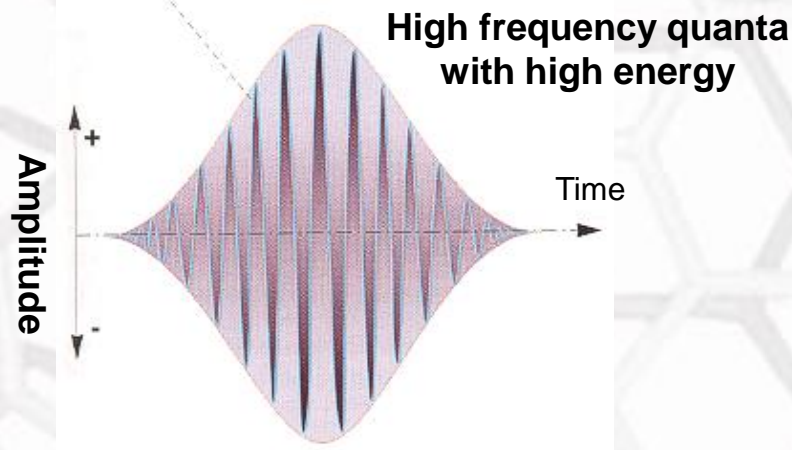


Max Planck's Idea

Light comes only in packets
or **quanta**,
which energy proportional
to their frequency, ν
or **angular frequency** ω .



Wave-packet



$$E = h \cdot \nu = \omega \cdot \hbar$$

where $h = 6.6261937 \cdot 10^{-37} \text{ J s}$
is **Planck's constant**

$\hbar = h/2\pi$ - reduced Planck constant

Planck's Formula

$$f(\omega, T) = \frac{\hbar \omega^3}{4\pi^2 c^2} \cdot \frac{1}{\exp(\hbar \omega / kT) - 1}$$

Bohr's Postulates (1913)



Niels Bohr
1885-1962

- ❑ The planetary model is correct, however, when an electron is in an "**allowed**" orbit it **does not radiate**.
- ❑ Conditions for "allowed" stationary orbit are:

$$L = m_e \cdot v \cdot r = n\hbar$$

where $n=1,2,3,\dots$,

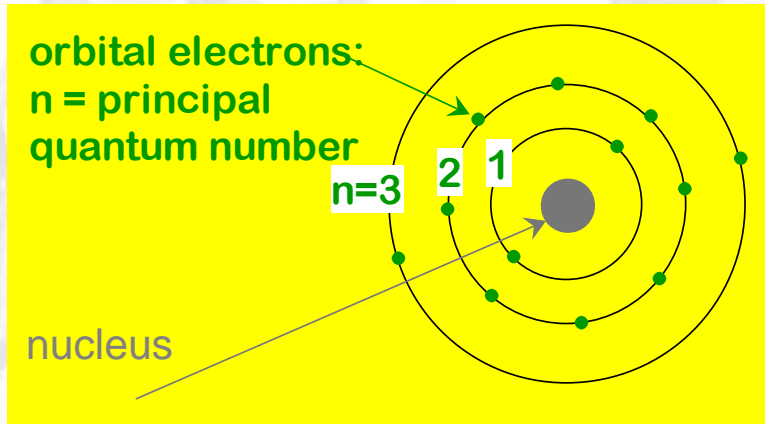
i.e. electron angular momentum is equal number of *Plank's constant*

- ❑ When electron "jumps" from one stationary orbit (**m** with energy E_m) to another (**n** and E_n) the radiation is **absorbed** ($E_m > E_n$) or **emitted** ($E_m < E_n$) in the form of a single **quantum** (photon) of electromagnetic energy:

$$E_n - E_m = \hbar \cdot \omega$$

Hydrogen Atom

Bohr's model was able to explain the **stability** of atoms as well as the emission spectrum of **hydrogen**.



Unfortunately, Bohr's model worked only for hydrogen. Thus final atomic model was yet to be developed.

$$m_e \frac{v^2}{r} = \frac{1}{4\pi\epsilon_0} \cdot \frac{Ze}{r^2}$$

$$m_e v r = n\hbar$$

$$r_n = 4\pi\epsilon_0 \frac{\hbar^2}{m_e Z e^2} \cdot n^2 \quad (n = 1, 2, 3, \dots)$$

$$n = 1 \quad r_{Bohr} = 0.529 \cdot 10^{-10} m$$

r_{Bohr} - Bohr radius

$$E = \frac{m_e v^2}{2} - \frac{1}{4\pi\epsilon_0} \cdot \frac{Ze^2}{r}$$

$$E = -\frac{1}{4\pi\epsilon_0} \cdot \frac{Ze^2}{2r}$$

$$E_n = -\left(\frac{1}{4\pi\epsilon_0}\right)^2 \cdot \frac{m_e Z e^4}{2\hbar^2} \cdot \frac{1}{n^2} \quad (n = 1, 2, 3, \dots)$$

$$E_n - E_m = \omega\hbar$$

$$\omega = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \cdot \frac{m_e Z e^4}{2\hbar^2} \cdot \left(\frac{1}{m^2} - \frac{1}{n^2}\right) = R \left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

$$R = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \cdot \frac{m_e Z e^4}{2\hbar^2} = 2.07 \cdot 10^{16} (2.0670687 \cdot 10^{16}) s^{-1} -$$

Rydberg const

Hypothesis of Prince Louis de Broglie



1892-1987
Nobel prize 1929

$$2\pi\omega = v$$
$$v = c/\lambda$$

In 1924 Louis de Broglie proposed that electrons have a wave nature. He also described the relationship between the wavelength of the wave and the mass and speed of the particle:

Photon energy: $E = h\omega/2\pi$

Photon impulse: $p = h/\lambda$

Eq. of real plane wave:

$$\xi = A \cdot \cos(\omega t - 2\pi x/\lambda)$$

Electron wave frequency: $\omega = 2\pi E/h$

Electron wave length: $\lambda = h/p$

De Broglie wave function for free particle:

$$\Psi = A \cdot \exp[(i2\pi/h)(p \cdot x - E \cdot t)]$$

The proposal has been experimentally (1927) confirmed and is one of the fundamental aspects of **Quantum Mechanics**.

Schrödinger Equation (1926)



Erwin Schrödinger
1887-1961

$$\Psi = A \exp [i2\pi/h \cdot (p \cdot x - E \cdot t)]$$

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} \cdot E \Psi; \quad \frac{\partial^2 \Psi}{\partial x^2} = \left(\frac{i}{\hbar}\right)^2 \cdot p^2 \Psi$$

$$E = \frac{1}{\Psi} i \hbar \frac{\partial \Psi}{\partial t}; \quad p^2 = -\frac{1}{\Psi} \hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$$

De Broglie Wave-function

As it was explained by Max Born $dP = |\Psi|^2 dV$ is a probability that particle could be detected inside volume dV .

$$E = \frac{p^2}{2m} + U;$$

U-is a potential Energy

$\int |\Psi|^2 dV = 1$ – standard conditions

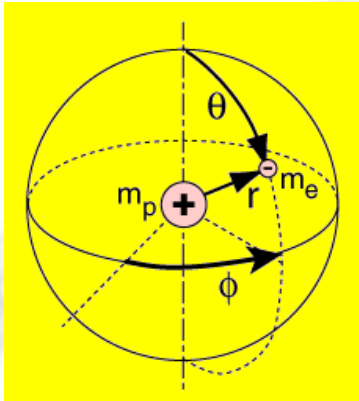
Energy conservation Law

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \Psi}{\partial x^2} + U \Psi = i \hbar \cdot \frac{\partial \Psi}{\partial t}$$

$$-\frac{\hbar^2}{2m} \cdot \Delta \psi + U \Psi = i \hbar \cdot \frac{\partial \Psi}{\partial t}$$

Famous Schrödinger Equation

Schrödinger Atom Model



if $\frac{\partial U}{\partial t} = 0$; stationary field

$$\Psi(x, y, z, t) = \psi(x, y, z) \exp[-i(E/\hbar)t]$$

$$-\frac{\hbar^2}{2m} \cdot \Delta \psi + U \psi = E \psi$$

$$\Delta \psi + \frac{2m}{\hbar^2} (E - U) \psi = 0;$$

$$\text{if } U = -\frac{1}{4\pi\epsilon_0} \cdot \frac{Ze_2}{r}$$

$$\Delta \psi + \frac{2m}{\hbar^2} \left(E + \frac{1}{4\pi\epsilon_0} \cdot \frac{Ze_2}{r} \right) \psi = 0;$$

or in polar coordinates

$$\frac{-\hbar^2}{2\mu} \frac{1}{r^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right] - U(r) \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi)$$

The solution of the Schrödinger Equation for the hydrogen atom is a formidable mathematical problem, but is of high fundamental **importance**. The **solution is managed by separating variables** so that the wave-function is represented as follows:

$$\Psi(r, \theta, \phi) = R(r)P(\theta)F(\phi)$$

n ← principal quantum number
 ℓ ← orbital quantum number
 m_ℓ ← magnetic quantum number

radial
colatitude
azimuthal equations

The separation leads to three equations for the three spatial variables, and their solutions give rise to three **quantum numbers** associated with the hydrogen energy levels.

The Principal Quantum Number

- The **principal quantum number** n arises from the solution of the **radial part** of the Schrödinger equation and describes the principle **energy level** of the electron.
- n is an integer that can range from 1 to infinity, with larger n corresponding to higher **energy orbital**
- The bound state energies of the electron in the hydrogen atom are given by:

$$E_n = \frac{-me^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} = \frac{-13.6eV}{n^2} \quad n = 1, 2, 3, \dots$$

In the notation (e.g. of the periodic table), the main shells of electrons are labeled **K**($n=1$), **L**($n=2$), **M**($n=3$), etc. based on the principal quantum number.

The Orbital Quantum Number

From constraints on the behavior of the wave-function in the *colatitude* equation arises a constant of the form:

$$l(l + 1) \quad \text{where } l = 0, 1, 2, 3, \dots, n - 1$$

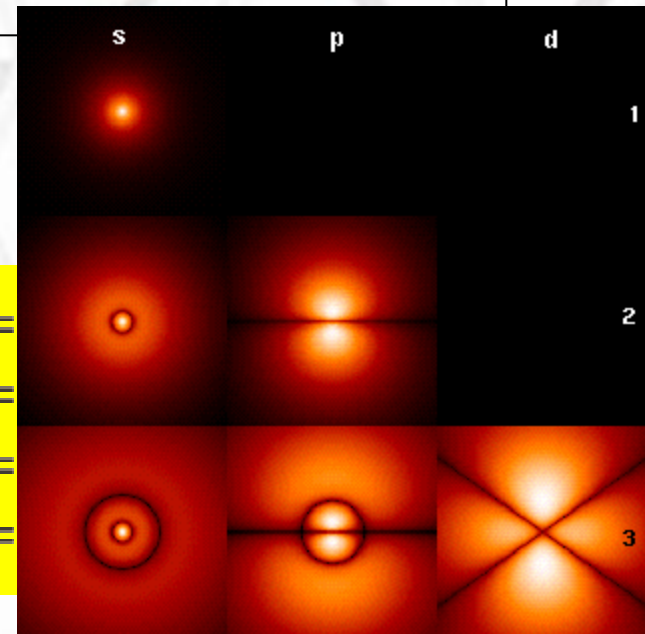
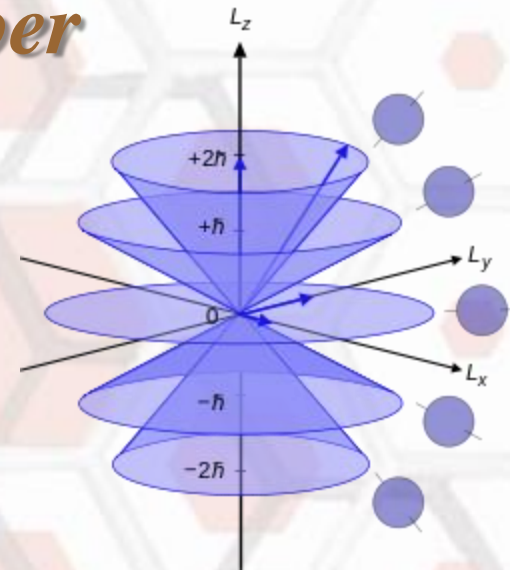
where **n** is the principal quantum number

This defines the **orbital quantum number, l**, which determines the magnitude of the *orbital angular momentum, L*, in the relationship:

$$L^2 = l(l + 1)\hbar^2$$

The orbital quantum number, **l**, is used as a part of the designation of atomic electron states in the spectroscopic notation

"sharp"	s	l =
"principal"	p	l =
"diffuse"	d	l =
"fundamental"	f	l =



The Magnetic Quantum Number

- From the *azimuthal equation* comes a third quantum number, m_l , with the constraint:

$$F(\phi) = Ae^{im_l\phi} \quad m_l = -l, -l+1, \dots, +l$$

- While the above azimuthal dependence of the wave-function only requires the quantum number to be an integer, the coupling with the colatitude equation further constrains that its absolute value to be less than or equal to the orbital quantum number, l . The direct implication of this quantum number is the *z-component of angular momentum*, L_z , is quantized according to:

$$L_z = m_l \hbar$$

m_l is called the **magnetic quantum number** because the *application of an external magnetic field causes a splitting of spectral lines called the Zeeman effect*.

Summary of Schrödinger Model

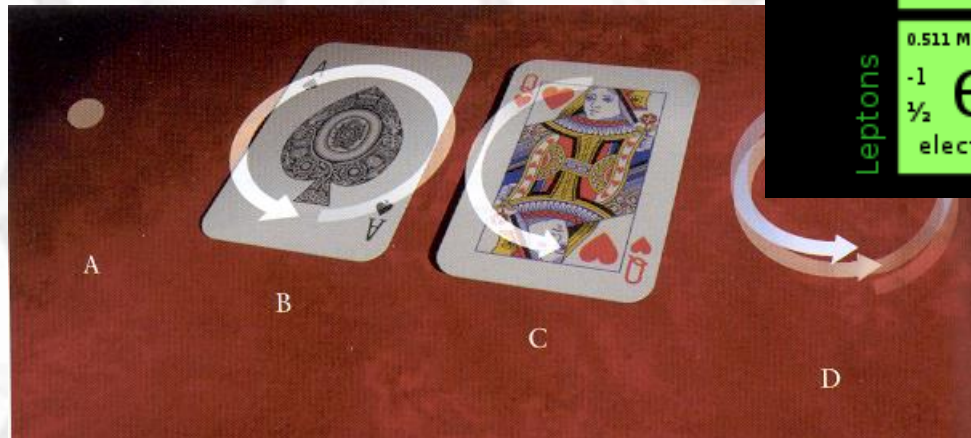
- The electron energy, E_n , is defined by **principle quantum number, n** .
- For each value of E_n (except E_1) one can find several wave-functions Ψ_{nlm} , with different values of **l** and **m_l** quantum numbers.
- For each n , number of states with different l and m_l equals:

$$\sum_{l=0}^{n-1} (2l + 1) = n^2$$

E_n	Ψ_{nlm}	Quantum numbers			E_n	Ψ_{nlm}	Quantum numbers		
		n	l	m_l			n	l	m_l
E_1	Ψ_{100}	1	0	0	E_3	Ψ_{300}	3	0	0
E_2	Ψ_{200} Ψ_{21-1} Ψ_{210} Ψ_{21+1}	2	0	0		Ψ_{31-1}	3	1	-1
						Ψ_{310}	3	1	0
						Ψ_{311}	3	1	+1
						Ψ_{32-2}	3	2	-2
						Ψ_{32-1}	3	2	-1
						Ψ_{320}	3	2	0
						Ψ_{321}	3	2	+1
						Ψ_{n322}	3	2	+2

Spin Quantum Number

Spin, is a particle **property**, which tells us what the different directions. A particle with **spin quantum number** m_s – looks same with different directions. A particle with $m_s=0$ – rotation a complete revolution. A particle with $m_s=1$ – it round half evolution. The particles exist which you evolutions, $m_s = 1/2$ to look the same!!!



	2.4 MeV $\frac{2}{3}$ $\frac{1}{2}$ u up	1.27 GeV $\frac{2}{3}$ $\frac{1}{2}$ c charm	171.2 GeV $\frac{2}{3}$ $\frac{1}{2}$ t top	0 0 1 Y photon
Quarks	4.8 MeV $-\frac{1}{3}$ $\frac{1}{2}$ d down	104 MeV $-\frac{1}{3}$ $\frac{1}{2}$ s strange	4.2 GeV $-\frac{1}{3}$ $\frac{1}{2}$ b bottom	0 0 1 g gluon
	< 2.2 eV 0 $\frac{1}{2}$ ν_e electron neutrino	< 0.17 MeV 0 $\frac{1}{2}$ ν_μ muon neutrino	< 15.5 MeV 0 $\frac{1}{2}$ ν_τ tau neutrino	91.2 GeV 0 1 Z weak force
Leptons	0.511 MeV -1 $\frac{1}{2}$ e electron	105.7 MeV -1 $\frac{1}{2}$ μ muon	1.777 GeV -1 $\frac{1}{2}$ τ tau	80.4 GeV ± 1 1 W weak force
				Bosons (Forces)

All the known particles in the Universe can be divided into two groups:

- Particles with $m_s = 1/2$ make the ***matter in the Universe***, e.g. e, p, n and etc.
- Particles with $m_s = 0, 1, 2$, give ***rise to force*** between the matter particles!!!

Spin Quantum Number (II)



Paul Dirac
1902-1984
Nobel Prize 1933

- A proper understanding of electron and other spin $\frac{1}{2}$ particles came 1928 from theory proposed by **Paul Dirac**, who for the first time combined both quantum mechanics and **special theory of relativity**. Thus spin is **quantum – relativistic property** of the particles.
- This theory also predicted that electron should have a partner: anti-electron or **positron**, which were discovered in 1932!!

Similarly to angular moment, spin projection on the z – direction is also quantized according to:

$$\mathbf{M}_{sz} = \mathbf{m}_s \hbar \quad \mathbf{m}_s = \mp 1/2$$

Thus an electron may have spin equals $+1/2$ or $-1/2$ and number of the electrons in atom with energy equals E_n may be not more than $2n^2$.

Pauli's Exclusion Principle



Wolfgang Pauli
1900-1958
Nobel Prize 1945

All particles with $\frac{1}{2}$ spin, i.e. the matter particles, obey what is called **Pauli's exclusion principle**:

*Two similar particles cannot exist in the same state, i.e. **only one** electron in atom can have a **given set of the four quantum numbers***

Principle	$n = 1, 2, 3, \dots$
Orbital	$l = 0, 1, 2, \dots, n-1$
Magnetic	$m_l = 0, \pm 1, \dots, \pm l$
Spin	$m_s = \pm 1/2$

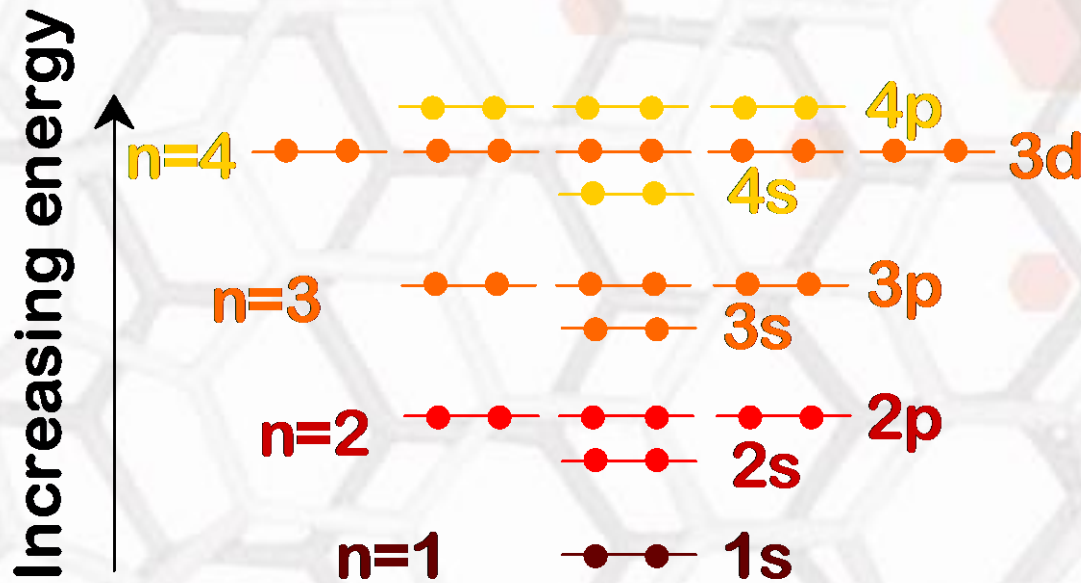
The number of Electrons in some Atom Shells

Principle Quantum Number, n	Shell Designation	Subshells	Number of states	Number of Electrons	
				Per Sub- shell	Per Shell
1	K	s	1	2	2
2	L	s	1	2	8
		p	3	6	
3	M	s	1	2	18
		p	3	6	
		d	5	10	
4	N	s	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

ELECTRON ENERGY STATES

Electrons...

- tend to occupy **lowest available energy state** or in other words, they fill quantum levels in order of increasing energy.
- electrons that occupy the outermost filled shell – the **valence electrons**- they are responsible for bonding and thus **material properties!!!**



STABLE ELECTRON CONFIGURATIONS

Stable electron configurations...

- have complete s and p sub-shells, i.e. to have **8** valence electrons –
- the *octet rule* !!
- this tends the atom to be un-reactive (stable) like an inert gasses.

Z	Element	Configuration
2	He	$1s^2$
10	Ne	$1s^2 2s^2 2p^6$
18	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
36	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

SURVEY of ELEMENTS

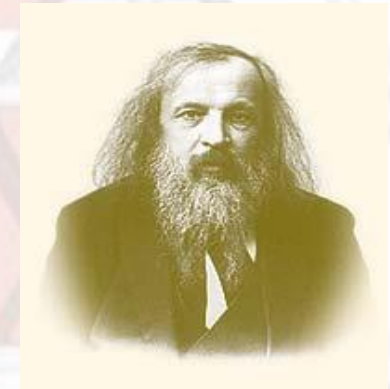
Element	K	L		M			N	
	1s	2s	2p	3s	3p	3d	4s	4p
1H	1	-	-	-	-	-	-	-
2He	2	-	-	-	-	-	-	-
3Li	2	1	-	-	-	-	-	-
4Be	2	2	-	-	-	-	-	-
5B	2	2	1	-	-	-	-	-
6C	2	2	2	-	-	-	-	-
7N	2	2	3	-	-	-	-	-
8O	2	2	4	-	-	-	-	-
9F	2	2	5	-	-	-	-	-
10Ne	2	2	6	-	-	-	-	-
11Na	2	8	1	-	-	-	-	-
12Mg	2	8	2	-	-	-	-	-
13Al	2	8	2	1	-	-	-	-
14Si	2	8	2	2	-	-	-	-
15P	2	8	2	3	-	-	-	-
16S	2	8	2	4	-	-	-	-
17Cl	2	8	2	5	-	-	-	-
18Ar	2	8	2	6	-	-	-	-
19K	2	8	8	-	1	-	-	-
20Ca	2	8	8	-	2	-	-	-
21Sc	2	8	8	1	2	-	-	-
22Ti	2	8	8	2	2	-	-	-
23V	2	8	8	3	2	-	-	-
24Cr	2	8	8	5	1	-	-	-
25Mn	2	8	8	5	2	-	-	-
26Fe	2	8	8	6	2	-	-	-
27Co	2	8	8	7	2	-	-	-
28Ni	2	8	8	8	2	-	-	-
29Cu	2	8	8	10	1	-	-	-
30Zn	2	8	8	10	2	-	-	-
31Ga	2	8	8	10	2	1	-	-
32Ge	2	8	8	10	2	2	-	-
33As	2	8	8	10	2	3	-	-
34Se	2	8	8	10	2	4	-	-
35Br	2	8	8	10	2	5	-	-
36Kr	2	8	8	10	2	6	-	-

Let us make columns of elements with similar **valence structure**

Periodic Table

Periodic table of the elements

period	group											13	14	15	16	17	18		
	1*											III _a	IV _a	V _a	VI _a	VII _a	0		
	Ia**																		
1	H																He		
2	Li	Be											B	C	N	O	F	Ne	
3	Na	Mg	III _b	IV _b	V _b	VI _b	VII _b	VIII _b	IX _b	X _b	XI _b	XII _b	Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cp	113 *** (Uut)	114 *** (Uuq)	115 *** (Uup)	116 *** (Uuh)		118 *** (Uuo)	
lanthanide series			6	58	59	60	61	62	63	64	65	66	67	68	69	70	71		
actinide series			7	90	91	92	93	94	95	96	97	98	99	100	101	102	103		



Dmitri Ivanovich Mendeleev
(1834-1907)

* Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC).

** Numbering system widely used, especially in the U.S., from the mid-20th century.

*** Discoveries of elements 113–116 and 118 are claimed but not confirmed. Element names and symbols in parentheses are temporarily assigned by IUPAC.

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- Elemental group indicates number of electrons available for bonding
For example: **IA** – Alkali metals (Li, Na, K..) – **one electron** in outermost occupied **s** subshell, eager to give up electron-very active with low melting points;
- VIIA** –Halogens (F, Br, Cl...) – **five electrons** in outermost occupied **p** subshell, need an electron to reach stable state – chemically active elements
- 0** - Inert gasses (he, Ne, Ar...) – have filled shells: chemically inactive

Conclusions

1. Now you know **physical interpretation** of the quantum numbers and that they are **naturally coming from the solution of the wave equation**:

The **principal quantum number**, symbolized as n can only have positive integer values ($n=1,2,..$)
As n increases, the electron is at a **higher potential energy** and is therefore less tightly bound to the nucleus. This is the only quantum number introduced by the Bohr model.

The **azimuthal quantum number**, symbolized l , is a quantum number for an atomic orbital that determines its **orbital angular momentum** and describes the **shape of the orbital** ($l=0,1,2,..n-1$).

The **magnetic quantum number** is the third of a set of quantum numbers is designated by the letter m , and refers, loosely, to the **direction of the angular momentum vector**. The magnetic quantum number m only affects the electron's energy if **it is in a magnetic field** because in the absence of one, all spherical harmonics corresponding to the different arbitrary values of m are equivalent ($m=-l, -l+1,..0,1, ..+l$).

The **spin quantum** is designated by the letter s . Naturally comes from the relativistic wave equation and correctly predicted the magnetic moment of electron, and at the same time treated the electron as a point particle ($s = 0,1, \pm 1/2$).

2. This numbers completely define **the electron structures of the elements** and allow to predict **type of bonds** which one can expect during the interaction between these elements.
3. We know that the **type of the atomic bonding** defines **materials properties**.